Sampling-Based Methods for Uncertainty and Sensitivity Analysis

Jon C. Helton
Dept 6849, MS 0779
Sandia National Laboratories
Albuquerque, NM 87185-0779
Ph: 505-284-4808
Fax: 505-844-2348
E-mail: jchelto@sandia.gov

Sampling-based approaches to uncertainty and sensitivity analysis are both effective and widely used [1-4]. Analyses of this type involve the generation and exploration of a mapping from uncertain analysis inputs to uncertain analysis results. The underlying idea is that analysis results $\mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x}), y_2(\mathbf{x}), \ldots, y_{nY}(\mathbf{x})]$ are functions of uncertain analysis inputs $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$. In turn, uncertainty in $\mathbf{x}$ results in a corresponding uncertainty in $\mathbf{y}(\mathbf{x})$. This leads to two questions: (i) What is the uncertainty in $\mathbf{y}(\mathbf{x})$ given the uncertainty in $\mathbf{x}$?, and (ii) How important are the individual elements of $\mathbf{x}$ with respect to the uncertainty in $\mathbf{y}(\mathbf{x})$? The goal of uncertainty analysis is to answer the first question, and the goal of sensitivity analysis is to answer the second question. In practice, the implementation of an uncertainty analysis and the implementation of a sensitivity analysis are very closely connected on both a conceptual and a computational level.

Implementation of a sampling-based uncertainty and sensitivity analysis involves five components: (i) Definition of distributions $D_1, D_2, \ldots, D_{nX}$ that characterize the uncertainty in the components $x_1, x_2, \ldots, x_{nX}$ of $\mathbf{x}$, (ii) Generation of a sample $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{nS}$ from the $\mathbf{x}$'s in consistency with the distributions $D_1, D_2, \ldots, D_{nX}$, (iii) Propagation of the sample through the analysis to produce a mapping $[\mathbf{x}_k, \mathbf{y}(\mathbf{x}_k)]$, $k = 1, 2, \ldots, nS$, from analysis inputs to analysis results, (iv) Presentation of uncertainty analysis results (i.e., approximations to the distributions of the elements of $\mathbf{y}$ constructed from the corresponding elements of $\mathbf{y}(\mathbf{x}_k)$, $k = 1, 2, \ldots, nS$), and (v) Determination of sensitivity analysis results (i.e., exploration of the mapping $[\mathbf{x}_k, \mathbf{y}(\mathbf{x}_k)]$, $k = 1, 2, \ldots, nS$). The five preceding steps will be discussed and illustrated with results from past analyses (e.g., [5-7]).

Definition of the distributions $D_1, D_2, \ldots, D_{nX}$ that characterize the uncertainty in the components $x_1, x_2, \ldots, x_{nX}$ of $\mathbf{x}$ is the most important part of a sampling-based uncertainty and sensitivity analysis as these distributions determine both the uncertainty in $\mathbf{y}$ and the sensitivity of $\mathbf{y}$ to the elements of $\mathbf{x}$. The distributions $D_1, D_2, \ldots, D_{nX}$ are typically defined through an expert review process [8-11], and their development can constitute a major analysis cost. A possible analysis strategy is to perform an initial exploratory analysis with rather crude definitions for $D_1, D_2, \ldots, D_{nX}$ and use sensitivity analysis to identify the most important analysis inputs; then, resources can be concentrated on characterizing the uncertainty in these inputs and a second presentation or decision-aiding analysis can be carried with these improved uncertainty characterizations.

Several sampling strategies are available, including random sampling, importance sampling, and Latin hypercube sampling [12, 13]. Latin hypercube sampling is very popular for use with computationally demanding models because its efficient stratification properties allow for the extraction of a large amount of uncertainty and sensitivity information with a relatively small sample size. In addition, effective correlation control procedures are available for use with Latin hypercube sampling [14, 15]. The popularity of Latin hypercube sampling recently led to the original article being designated a *Technometrics* classic in experimental design [16].

Propagation of the sample through the analysis to produce the mapping $[\mathbf{x}_k, \mathbf{y}(\mathbf{x}_k)]$, $k = 1, 2, \ldots, nS$, from analysis inputs to analysis results is often the most computationally demanding part of a sampling-based uncertainty and sensitivity analysis. The details of this propagation are analysis specific and can range from very simple for analyses that involve a single model to very complicated for large analyses that involve complex systems of linked models [7, 17].

Presentation of uncertainty analysis results is generally straight forward and involves little more than displaying the results associated with the already calculated mapping $[\mathbf{x}_k, \mathbf{y}(\mathbf{x}_k)]$, $k = 1, 2, \ldots, nS$. Presentation possibilities include means and standard deviations, density functions, cumulative distribution functions (CDFs), complementary cumulative distribution functions (CCDFs), and box plots [2, 13]. Presentation formats such as CDFs, CCDFs and box plots are usually preferable to means and standard deviations because of the large amount of uncertainty information that is lost in the calculation of means and standard deviations.

Determination of sensitivity analysis results is usually more demanding than the presentation of uncertainty analysis results due to the need to actually explore the mapping $[\mathbf{x}_k, \mathbf{y}(\mathbf{x}_k)]$, $k = 1, 2, \ldots, nS$, to assess the effects of individual components of $\mathbf{x}$ on the components of $\mathbf{y}$. Available sensitivity analysis procedures include examination of scatterplots, regression analysis, correlation and partial correlation analysis, stepwise regression analysis, rank transformations to linearize monotonic relationships, identification of nonmonotonic patterns, and identification of nonrandom patterns [2-4, 18, 19].

Sampling-based uncertainty and sensitivity analysis is widely used, and as a result, is a fairly mature area of study. However, there still remain a number of important challenges and areas for additional study. For example, there is a need for sensitivity analysis procedures that are more effective at revealing nonlinear relations than those currently in use. Possibilities include procedures based on nonparametric regression [20-22], the two-dimensional Kolmogorov-Smirnov test [23-25], tests for nonmonotone relations [26], tests for nonrandom patterns [27-31], and complete variance decomposition [32, 33]. As another example, sampling-based procedures for uncertainty and sensitivity analysis usually use probability as the model, or representation, for uncertainty. However, when limited information is available with which to characterize uncertainty, probabilistic characterizations can give the appearance of more knowledge than is really present. Alternative representations for uncertainty such as evidence theory and possibility theory merit consideration for their potential to represent uncertainty in situations where little information is available [34, 35]. Finally, a significant challenge is the education of potential users of uncertainty and sensitivity analysis about (i) the importance of such analyses and their role in both large and small analyses, (ii) the need for an appropriate separation of aleatory and epistemic uncertainty in the conceptual and computational implementation of analyses of complex systems [36-40], (iii) the need for a clear conceptual view of what an analysis is intended to represent and a computational design that is consistent with that view [41], and (iv) the importance of avoiding deliberately conservative assumptions if meaningful uncertainty and sensitivity analysis results are to be obtained.

References

1. Iman, R.L. 1992. "Uncertainty and Sensitivity Analysis for Computer Modeling Applications," *Reliability Technology - 1992, The Winter Annual Meeting of the American Society of Mechanical Engineers, Anaheim, California, November 8-13, 1992*. Eds. T.A. Cruse. Vol. 28. New York, NY: American Society of Mechanical Engineers, Aerospace Division. 153-168.
2. Helton, J.C. 1993. "Uncertainty and Sensitivity Analysis Techniques for Use in Performance Assessment for Radioactive Waste Disposal," *Reliability Engineering and System Safety*. Vol. 42, no. 2-3, pp. 327-367.
3. Hamby, D.M. 1994. "A Review of Techniques for Parameter Sensitivity Analysis of Environmental Models," *Environmental Monitoring and Assessment*. Vol. 32, no. 2, pp. 135-154.
4. Blower, S.M. and H. Dowlatabadi. 1994. "Sensitivity and Uncertainty Analysis of Complex Models of Disease Transmission: an HIV Model, as an Example," *International Statistical Review*. Vol. 62, no. 2, pp. 229-243.
5. Helton, J.C., D.R. Anderson, H.-N. Jow, M.G. Marietta, and G. Basabilvazo. 1999. "Performance Assessment in Support of the 1996 Compliance Certification Application for the Waste Isolation Pilot Plant," *Risk Analysis*. Vol. 19, no. 5, pp. 959 - 986.
6. Helton, J.C. 1999. "Uncertainty and Sensitivity Analysis in Performance Assessment for the Waste Isolation Pilot Plant," *Computer Physics Communications*. Vol. 117, no. 1-2, pp. 156-180.
7. Helton, J.C. and M.G. Marietta. 2000. "Special Issue: The 1996 Performance Assessment for the Waste Isolation Pilot Plant," *Reliability Engineering and System Safety*. Vol. 69, no. 1-3, pp. 1-451.
8. Hora, S.C. and R.L. Iman. 1989. "Expert Opinion in Risk Analysis: The NUREG-1150 Methodology," *Nuclear Science and Engineering*. Vol. 102, no. 4, pp. 323-331.
9. Thorne, M.C. and M.M.R. Williams. 1992. "A Review of Expert Judgement Techniques with Reference to Nuclear Safety," *Progress in Nuclear Safety*. Vol. 27, no. 2-3, pp. 83-254.
10. Budnitz, R.J., G. Apostolakis, D.M. Boore, L.S. Cluff, K.J. Coppersmith, C.A. Cornell, and P.A. Morris. 1998. "Use of Technical Expert Panels: Applications to

Probabilistic Seismic Hazard Analysis," *Risk Analysis*. Vol. 18, no. 4, pp. 463-469.

11. McKay, M. and M. Meyer. 2000. "Critique of and Limitations on the use of Expert Judgements in Accident Consequence Uncertainty Analysis," *Radiation Protection Dosimetry*. Vol. 90, no. 3, pp. 325-330.
12. McKay, M.D., R.J. Beckman, and W.J. Conover. 1979. "A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code," *Technometrics*. Vol. 21, no. 2, pp. 239-245.
13. Helton, J.C. and F.J. Davis. 2003. "Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems," *Reliability Engineering and System Safety*. Vol. 81, no. 1, pp. 23-69.
14. Iman, R.L. and W.J. Conover. 1982. "A Distribution-Free Approach to Inducing Rank Correlation Among Input Variables," *Communications in Statistics: Simulation and Computation*. Vol. B11, no. 3, pp. 311-334.
15. Iman, R.L. and J.M. Davenport. 1982. "Rank Correlation Plots for Use with Correlated Input Variables," *Communications in Statistics: Simulation and Computation*. Vol. B11, no. 3, pp. 335-360.
16. Morris, M.D. 2000. "Three Technometrics Experimental Design Classics," *Technometrics*. Vol. 42, no. 1, pp. 26-27.
17. Breeding, R.J., J.C. Helton, E.D. Gorham, and F.T. Harper. 1992. "Summary Description of the Methods Used in the Probabilistic Risk Assessments for NUREG-1150," *Nuclear Engineering and Design*. Vol. 135, no. 1, pp. 1-27.
18. Helton, J.C. and F.J. Davis. 2000. "Sampling-Based Methods for Uncertainty and Sensitivity Analysis," *Sensitivity Analysis*. A. Saltelli, K. Chan, and E.M. Scott (eds). New York, NY: Wiley. pp. 101-153.
19. Helton, J.C. and F.J. Davis. 2002. "Illustration of Sampling-Based Methods for Uncertainty and Sensitivity Analysis," *Risk Analysis*. Vol. 22, no. 3, pp. 691-622.
20. Hastie, T.J. and R.J. Tibshirani. 1990. *Generalized Additive Models*. London: Chapman & Hall.
21. Simonoff, J.S. 1996. *Smoothing Methods in Statistics*. New York: Springer-Verlag.
22. Bowman, A.W. and A. Azzalini. 1997. *Applied Smoothing Techniques for Data Analysis*. Oxford: Clarendon.
23. Peacock, J.A. 1983. "Two-Dimensional Goodness-Of-Fit Testing in Astronomy," *Monthly Notices of the Royal Astronomical Society*. Vol. 202, no. 2, pp. 615-627.
24. Fasano, G. and A. Franceschini. 1987. "A Multidimensional Version of the Kolmogorov-Smirnov Test," *Monthly Notices of the Royal Astronomical Society*. Vol. 225, no. 1, pp. 155-170.
25. Garvey, J.E., E.A. Marschall, and R. Wright, A. 1998. "From Star Charts to Stoneflies: Detecting Relationships in Continuous Bivariate Data," *Ecology*. Vol. 79, no. 2, pp. 442-447.
26. Hora, S.C. and J.C. Helton. 2003. "A Distribution-Free Test for the Relationship Between Model Input and Output when Using Latin Hypercube Sampling," *Reliability Engineering and System Safety*. Vol. 79, no. 3, pp. 333-339.
27. Ripley, B.D. 1979. "Tests of "Randomness" for Spatial Point Patterns," *Journal of the Royal Statistical Society*. Vol. 41, no. 3, pp. 368-374.

28. Diggle, P.J. and T.F. Cox. 1983. "Some Distance-Based Tests of Independence for Sparsely-Sampled Multivariate Spatial Point Patterns," *International Statistical Review*. Vol. 51, no. 1, pp. 11-23.
29. Zeng, G. and R.C. Dubes. 1985. "A Comparison of Tests for Randomness," *Pattern Recognition*. Vol. 18, no. 2, pp. 191-198.
30. Assunçao, R. 1994. "Testing Spatial Randomness by Means of Angles," *Biometrics*. Vol. 50, pp. 531-537.
31. Kleijnen, J.P.C. and J.C. Helton. 1999. "Statistical Analyses of Scatterplots to Identify Important Factors in Large-Scale Simulations, 1: Review and Comparison of Techniques," *Reliability Engineering and System Safety*. Vol. 65, no. 2, pp. 147-185.
32. Saltelli, A., S. Tarantola, and K.P.-S. Chan. 1999. "A Quantitative Model-Independent Method for Global Sensitivity Analysis of Model Output," *Technometrics*. Vol. 41, no. 1, pp. 39-56.
33. Li, G., C. Rosenthal, and H. Rabitz. 2001. "High-Dimensional Model Representations," *The Journal of Physical Chemistry*. Vol. 105, no. 33, pp. 7765-7777.
34. Klir, G.J. and M.J. Wierman. 1999. *Uncertainty-Based Information*, New York, NY: Physica-Verlag.
35. Helton, J.C., J.D. Johnson, and W.L. Oberkampf. "An Exploration of Alternative Approaches to the Representation of Uncertainty in Model Predictions," *Reliability Engineering and System Safety (to appear)*.
36. Apostolakis, G. 1990. "The Concept of Probability in Safety Assessments of Technological Systems," *Science*. Vol. 250, no. 4986, pp. 1359-1364.
37. Helton, J.C. 1994. "Treatment of Uncertainty in Performance Assessments for Complex Systems," *Risk Analysis*. Vol. 14, no. 4, pp. 483-511.
38. Hoffman, F.O. and J.S. Hammonds. 1994. "Propagation of Uncertainty in Risk Assessments: The Need to Distinguish Between Uncertainty Due to Lack of Knowledge and Uncertainty Due to Variability," *Risk Analysis*. Vol. 14, no. 5, pp. 707-712.
39. Paté-Cornell, M.E. 1996. "Uncertainties in Risk Analysis: Six Levels of Treatment," *Reliability Engineering and System Safety*. Vol. 54, no. 2-3, pp. 95-111.
40. Helton, J.C. 1997. "Uncertainty and Sensitivity Analysis in the Presence of Stochastic and Subjective Uncertainty," *Journal of Statistical Computation and Simulation*. Vol. 57, no. 1-4, pp. 3-76.
41. Helton, J.C. 2001. "Mathematical and Numerical Approaches in Performance Assessment for Radioactive Waste Disposal: Dealing with Uncertainty," *Etude pour la Faisabilité des Stochazes de Déchets Radioactifs, Actes des Journées Scientifiques ANDRA, Nancy, 7, 8, et 9 decembré 1999*. Les Ulis cedex A, France: EDP Sciences. 59-90.